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| | | | |
|---|---|---|---|
| NEWS | 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS | 2 | JAN 02 | STN pricing information for 2008 now available |
| NEWS | 3 | JAN 16 | CAS patent coverage enhanced to include exemplified prophetic substances |
| NEWS | 4 | JAN 28 | USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats |
| NEWS | 5 | JAN 28 | MARPAT searching enhanced |
| NEWS | 6 | JAN 28 | USGENE now provides USPTO sequence data within 3 days of publication |
| NEWS | 7 | JAN 28 | TOXCENTER enhanced with reloaded MEDLINE segment |
| NEWS | 8 | JAN 28 | MEDLINE and LMEDLINE reloaded with enhancements |
| NEWS | 9 | FEB 08 | STN Express, Version 8.3, now available |
| NEWS | 10 | FEB 20 | PCI now available as a replacement to DPCI |
| NEWS | 11 | FEB 25 | IFIREF reloaded with enhancements |
| NEWS | 12 | FEB 25 | IMSPRODUCT reloaded with enhancements |
| NEWS | 13 | FEB 29 | WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification |
| NEWS | 14 | MAR 31 | IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats |
| NEWS | 15 | MAR 31 | CAS REGISTRY enhanced with additional experimental spectra |
| NEWS | 16 | MAR 31 | CA/CAplus and CASREACT patent number format for U.S. applications updated |
| NEWS | 17 | MAR 31 | LPCI now available as a replacement to LDPCI |
| NEWS | 18 | MAR 31 | EMBASE, EMBAL, and LEMBASE reloaded with enhancements |
| NEWS | 19 | APR 04 | STN AnaVist, Version 1, to be discontinued |

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

| | |
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| NEWS IPC8 | For general information regarding STN implementation of IPC 8 |

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

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=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                             ENTRY    SESSION
FULL ESTIMATED COST                                           0.21       0.21

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DICTIONARY FILE UPDATES:   3 APR 2008  HIGHEST RN 1012038-13-9

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Uploading C:\Program Files\Stnexp\Queries\10579836.str
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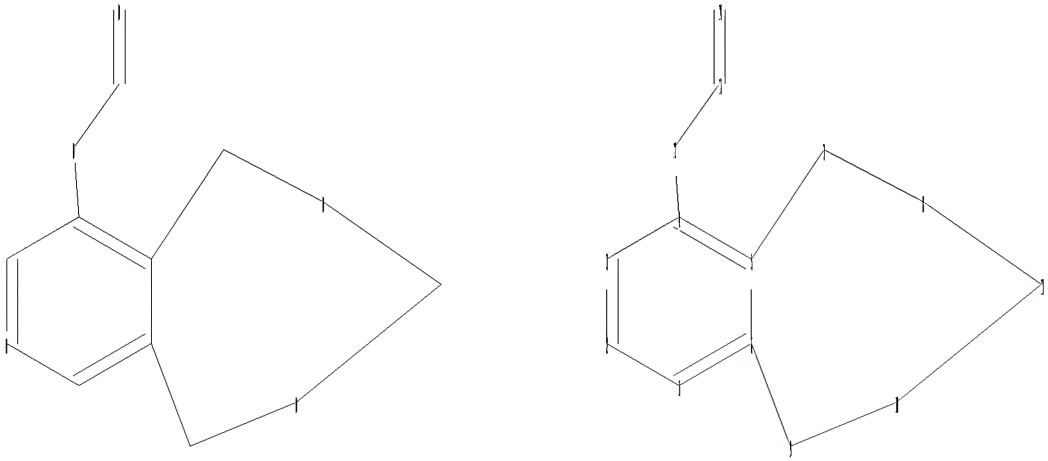

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chain nodes :
12  13  14
ring nodes :
1  2  3  4  5  6  7  8  9  10  11
chain bonds :
4-12  12-13  13-14
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-11  9-10  10-11
exact/norm bonds :
4-12  12-13  13-14
exact bonds :
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5-7  6-9  7-8  8-11  9-10  10-11
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:CLASS  13:CLASS  14:CLASS

L1      STRUCTURE UPLOADED

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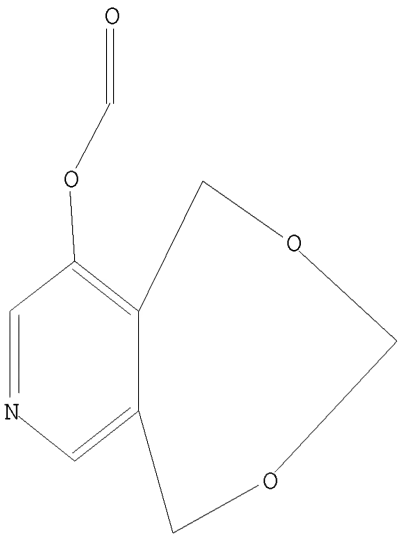
L1              STR




Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -        7 TO ITERATE

100.0% PROCESSED        7 ITERATIONS                                4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:             7 TO      298
PROJECTED ANSWERS:                4 TO      200

L2            4 SEA SSS SAM L1

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FULL SCREEN SEARCH COMPLETED -       89 TO ITERATE

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100.0% PROCESSED       89 ITERATIONS                              27 ANSWERS
SEARCH TIME: 00.00.01

L3           27 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     178.36     178.57

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FILE LAST UPDATED: 3 Apr 2008  (20080403/ED)

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=> s l3 full
L4           20 L3

=> s l3/prep full
             20 L3
        4552880 PREP/RL
L5           17 L3/PREP
                  (L3 (L) PREP/RL)

=> d ibib abs hitstr tot
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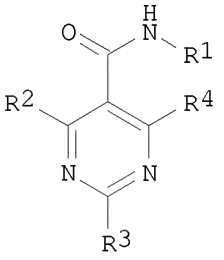
L5 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:165553 CAPLUS
DOCUMENT NUMBER: 146:206335
TITLE: Preparation of pyrimidinecarboxamides as CXCR2 receptor antagonists for the treatment of inflammation
INVENTOR(S): Baughman, Theodore A.; Boyce, Jim P.; Darwish, Ihab S.; Howbert, J. Jeffry; Ihle, Nathan C.; Jackson, Randy W.; Jeffrey, Scott C.; Maeda, Dean; Yager, Kraig M.
PATENT ASSIGNEE(S): Ucb SA, UK
SOURCE: U.S., 32pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|
| US 7176310 | B1 | 20070213 | US 2003-407870 | | 20030404 |
| PRIORITY APPLN. INFO.: | | | US 2002-371265P | P | 20020409 |

OTHER SOURCE(S): MARPAT 146:206335
GI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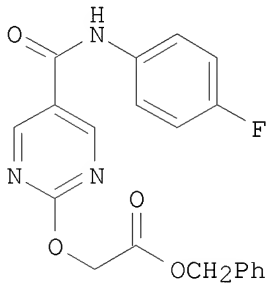
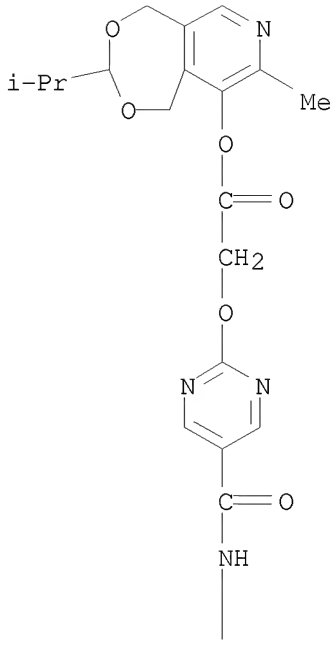

II

AB Title compds. I [wherein R1 = aralkyl or aryl; R2 = H or NH2; R3 = aryloxy, arylsulfinyl, amino, etc.; R4 = H, halo or alkyl, with limitations] and their stereoisomers, pharmaceutically acceptable salts or solvates thereof, which are useful as chemokine CXCR2 receptor antagonist and anti-inflammatory agents (no data), were prepared Thus, compound II was obtained in 30% yield by condensation of the corresponding 2-methylsulfinylpyrimidine (preparation given) with benzyl glycolate.

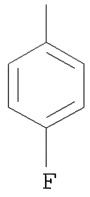
IT 923292-04-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinecarboxamide derivs. as CXCR2 receptor antagonists for treatment of inflammation)

RN 923292-04-0 CAPLUS
CN Acetic acid, 2-[[5-[[(4-fluorophenyl)amino]carbonyl]-2-pyrimidinyl]oxy]-, 1,5-dihydro-8-methyl-3-(1-methylethyl)[1,3]dioxepino[5,6-c]pyridin-9-yl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:472161 CAPLUS
DOCUMENT NUMBER: 143:7535
TITLE: Manufacture of vitamin B6 and related 9-acyloxy-1,5-dihydro-8-methylpyrido[3,4-e][1,3]dioxepins
INVENTOR(S): Fischesser, Jocelyn; Fritsch, Helmut; Gum, Andrew George; Karge, Reinhard; Keuper, Ralf
PATENT ASSIGNEE(S): DSM IP Assets B. V., Neth.
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005049618 | A1 | 20050602 | WO 2004-EP12655 | 20041109 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1685133 | A1 | 20060802 | EP 2004-818764 | 20041109 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS | | | | |
| CN 1882592 | A | 20061220 | CN 2004-80034214 | 20041109 |
| JP 2007511558 | T | 20070510 | JP 2006-540247 | 20041109 |
| US 20070072254 | A1 | 20070329 | US 2006-579836 | 20060608 |
| PRIORITY APPLN. INFO.: | | | DE 2003-10353999 A | 20031119 |
| | | | WO 2004-EP12655 W | 20041109 |
| OTHER SOURCE(S): | CASREACT 143:7535; MARPAT 143:7535 | | | |

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

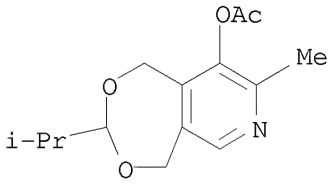
AB A process for manufacturing a 3-un-, 3-mono- or 3,3-disubstituted 9-acyloxy-1,5-dihydro-8-methylpyrido[3,4-e] [1,3]dioxepin I [R2, R3 = H, C1-4-alkyl C2-4-alkenyl; R4 = C1-4-alkyl, C1-4-haloalkyl, Ph-(C1-4-alkyl), Ph; CR2R3 = C4-6-cycloalkylidene] and optionally for manufacturing pyridoxine involves performing an addition reaction between a 4-methyl-5-alkoxy-oxazole II [R1 = C1-4-alkyl] and a 2-un-, 2-mono- or 2,2-disubstituted 4,7-dihydro-1,3-dioxepin III in the substantial absence of a solvent and a catalyst to give a product mixture consisting essentially of the appropriate Diels-Alder adduct IV in a major proportion and the appropriate 3-un-, 3-mono- or 3,3-disubstituted 1,5-dihydro-8-methylpyrido[3,4-e][1,3]dioxepin-9-ol V in a minor proportion, removal of a substantial proportion of the unreacted oxazole and dioxepin starting materials from the product mixture by distillation under reduced pressure, addition of a substantially anhydrous organic acid to said product mixture and rearrangement of the Diels-Alder adduct IV to further V in the presence of said

substantially anhydrous organic acid with removal of the generated alkanol by distillation under reduced pressure, and acylation of the resultingly enriched quantity of V with an added carboxylic acid anhydride, (R4CO)2O to produce the desired I, and optionally converting this so-manufactured acylation product I to pyridoxine by acid hydrolysis for achieving deprotection and deacylation. Pyridoxine [VI] is a well known form of vitamin B6 with well established utility.

IT 92671-67-5P, 9-Acetoxy-1,5-Dihydro-3-isopropyl-8-methylpyrido[3,4-e][1,3]dioxepin
RL: SPN (Synthetic preparation); PREP (Preparation)
(manufacture of vitamin B6 and related 9-acyloxy-1,5-dihydro-8-methylpyrido[3,4-e][1,3]dioxepins)

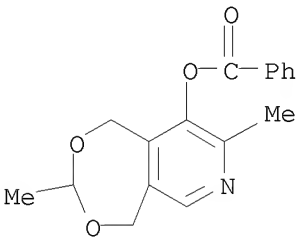
RN 92671-67-5 CAPLUS

CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-8-methyl-3-(1-methylethyl)-, acetate (ester) (9CI) (CA INDEX NAME)

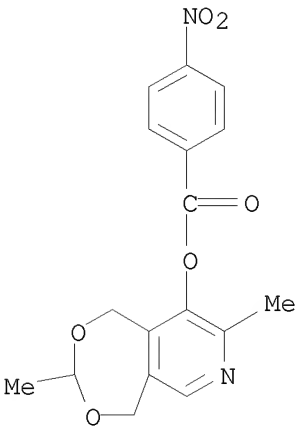



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:981764 CAPLUS
DOCUMENT NUMBER: 138:287060
TITLE: Crystal structure of seven-membered acetals with furan and pyridine planar fragments
AUTHOR(S): Fedorenko, V. Yu.; Lodochnikova, O. A.; Petukhov, A. S.; Kataeva, O. N.; Litvinov, I. A.; Shtyrlin, Yu. G.; Klimovitskii, E. N.
CORPORATE SOURCE: A.M. Butlerov Chemical Research Institute, Kazan State University, Kazan, 420008, Russia
SOURCE: Journal of Molecular Structure (2003), 644(1-3), 89-96
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB X-ray structure investigation of fused seven-membered acetals based on vitamin B6 and 3,4-bis(hydroximethyl)furan have been performed. Mols. adopt chair conformations with equatorial position of substituents at acetal carbons; the geometry of acetal cycles resembles that of related seven-membered phthalylacetals. Stereochem. of the tetracyclic adduct of furan-containing acetal with maleic anhydride was also investigated. The product exhibits endo-exo configuration with appreciably distorted seven-membered chair-like conformation.
IT 451461-88-4P 505074-22-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystallog. of)
RN 451461-88-4 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,8-dimethyl-, benzoate (ester) (9CI) (CA INDEX NAME)




RN 505074-22-6 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,8-dimethyl-, 4-nitrobenzoate (ester) (9CI) (CA INDEX NAME)



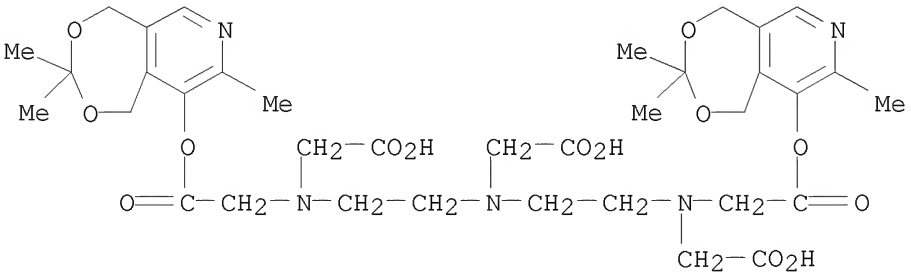

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:103940 CAPLUS
DOCUMENT NUMBER: 136:334219
TITLE: Studies on the synthesis, relaxivity and liver-targeting of DTPA-pyridoxol ester gadolinium complexes
AUTHOR(S): Ding, Xiong-jun; Zhuo, Ren-xi; Fu, Gong-cheng
CORPORATE SOURCE: Key Lab. of Biomedical Polymer Materials, Ministry of Education; Department of Chemistry, Wuhan University, Wuhan, 43--72, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2002), 23(1), 49-52
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 136:334219

AB Several new DTPA-pyridoxol ester ligands ROOCCH2N(CH2COOH)CH2CH2N(CH2COOH)CH2CH2N(CH2COOH)CH2COOR were synthesized by reacting diethylenetriaminepentaacetic anhydride (DTPAA) with pyridoxol (R) derivs. Their gadolinium complexes were also prepared Their T1 relaxivities in water were measured. The 99Tc-labeled combination radioactivity experiment with liver cells and kidney cells of mice showed that two ligands possessed an excellent liver-targeting property. The results of animal MR imaging experiment further confirmed that the signals in liver were obviously strengthened after injection of their complexes.

IT 412939-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reactant; preparation, T1 relaxivity, and liver-targeting properties of gadolinium DTPA-pyridoxol ester complexes in 99Tc-labeled combination radioactivity expts.)

RN 412939-75-4 CAPLUS
CN Glycine, N,N-bis[2-[(carboxymethyl)[2-[(1,5-dihydro-3,3,8-trimethyl[1,3]dioxepino[5,6-c]pyridin-9-yl)oxy]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

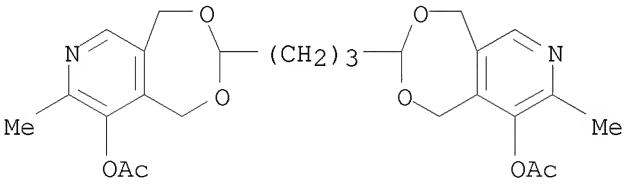


L5 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:106715 CAPLUS
DOCUMENT NUMBER: 126:186065
TITLE: Chemistry of 1,3-dioxepins. XI. Bis(4,7-dihydro-1,3-dioxepin) approach to pyridoxine intermediates 1,5-dihydro-8-methyl-3H-[1,3]dioxepino[5,6-c]pyridin-9-ols
AUTHOR(S): Dumic, Miljenko; Vinkovic, Mladen; Jadrijevic-Mladar Takac, Milena; Butula, Ivan
CORPORATE SOURCE: PLIVA-Research Institute, Zagreb, HR-10000, Croatia
SOURCE: Croatica Chemica Acta (1996), 69(4), 1561-1576
CODEN: CCACAA; ISSN: 0011-1643
PUBLISHER: Croatian Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

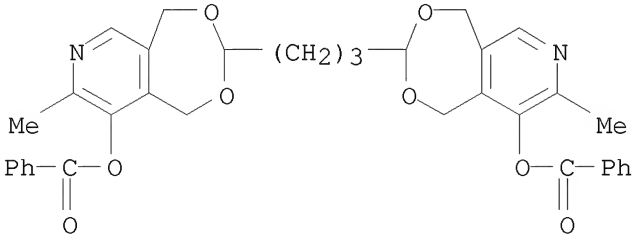
AB The novel pyridoxine intermediates, bis-dioxepino[5,6-c]pyridin-9-ols have been synthesized starting from bis-(4,7-dihydro-1,3-dioxepins). Their constitution and configuration has been confirmed by single-crystal X-ray diffractions.

IT 187467-71-6P 187467-73-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 187467-71-6 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 3,3'-(1,3-propanediyl)bis[1,5-dihydro-8-methyl-, diacetate (ester) (9CI) (CA INDEX NAME)

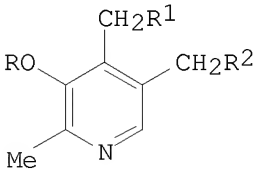



RN 187467-73-8 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 3,3'-(1,3-propanediyl)bis[1,5-dihydro-8-methyl-, dibenzoate (ester) (9CI) (CA INDEX NAME)




REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:455657 CAPLUS
DOCUMENT NUMBER: 97:55657
ORIGINAL REFERENCE NO.: 97:9369a,9372a
TITLE: Heterogeneous condensation of lauroyl chloride with some pyridine derivatives in the presence of alkali
AUTHOR(S): Koruncev, Dimitar; Coric, Miljenko; Rota, Hrvatinka; Miric, Ljubomir
CORPORATE SOURCE: Zagreb, Yugoslavia
SOURCE: Farmaceutski Glasnik (1982), 38(3), 73-5
CODEN: FAGLAI; ISSN: 0014-8202
DOCUMENT TYPE: Journal
LANGUAGE: Serbo-Croatian
GI

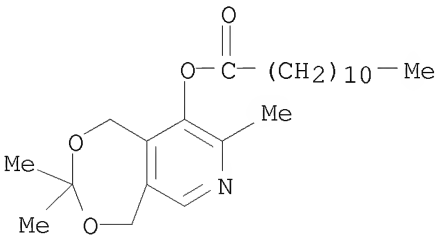


I

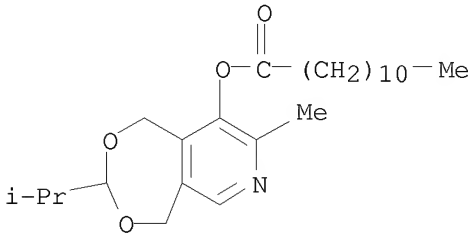
AB Acylation of pyridoxine derivs. I (R = H; R1 = R2 = OAc, Br, NHC6H4CF3-3; R1 = OMe, R2 = OAc; R1R2 = O2CHCHMe2, O2CMe2) with Me(CH2)10COCl in C6H6, PhMe or petroleum ether containing 1 equivalent solid or aqueous alkali at room temperature gave .apprx.80% I [R = Me(CH2)10CO; same R1, R2].

IT 82470-52-8P 82483-56-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

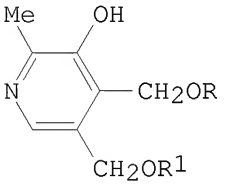
RN 82470-52-8 CAPLUS
CN Dodecanoic acid, 1,5-dihydro-3,3,8-trimethyl[1,3]dioxepino[5,6-c]pyridin-9-yl ester (CA INDEX NAME)



RN 82483-56-5 CAPLUS
CN Dodecanoic acid, 1,5-dihydro-8-methyl-3-(1-methylethyl)[1,3]dioxepino[5,6-c]pyridin-9-yl ester (CA INDEX NAME)

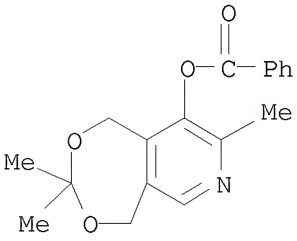


L5 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:79353 CAPLUS
DOCUMENT NUMBER: 96:79353
ORIGINAL REFERENCE NO.: 96:12893a,12896a
TITLE: Stability, bactericidal activity, vitamin B6 activity and gastrointestinal absorption of benzoic acid esters of pyridoxine
AUTHOR(S): Mizuno, Nobuyasu; Fukumoto-Hato, Miyako; Matsumoto-Yoshino, Miyuki; Morita, Emiko
CORPORATE SOURCE: Fac. Pharm. Sci., Mukogawa Women's Univ., Hyogo, 663, Japan
SOURCE: Journal of Nutritional Science and Vitaminology (1981), 27(3), 165-75
CODEN: JNSVA5; ISSN: 0301-4800
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

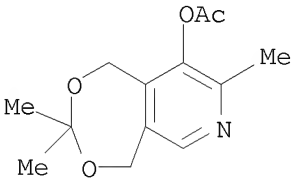


I, R=Bz, $R^1$=H
II, R=H, $R^1$=Bz

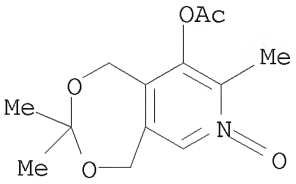
AB α4-O-Benzoyl pyridoxine (PN-4'MB)(I) was synthesized; PN-4'MB and α5-O-benzoyl pyridoxine (PN-5'MB)(II) obeyed apparent first-order kinetics when hydrolyzed in 10% aqueous acetone solution at pH 1-4. At pH 1-7, PN-4'MB was hydrolyzed 10 times faster than PN-5'MB. At pH 7-12, an interconversion between the 2 derivs. was observed Both were bactericidal against Escherichia coli and Bacillus subtilis and prevented severe convulsions induced in mice by 4'-methoxypyridoxine, a potent antagonist of vitamin B6. PN-4'MB was hydrolyzed by rat liver homogenates more easily than PN-5'MB. The metabolite of both in man was identified as 4'-pyridoxic acid, a principal metabolite of pyridoxine, by high-performance liquid chromatog. The amount of urinary excretion of 4'-pyridoxic acid in 10 h after oral administration of PN-4'MB or PN-5'MB was as large as that after pyridoxine. Thus, I and II, when used as an ointment or cosmetic preservative, appear to be hydrolyzed by skin enzymes and exhibit bactericidal and vitamin B6 activities.
IT 14210-76-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deketalization of)
RN 14210-76-5 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, benzoate (ester) (8CI, 9CI) (CA INDEX NAME)



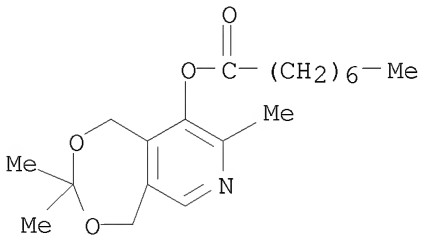
L5 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:89958 CAPLUS
DOCUMENT NUMBER: 84:89958
ORIGINAL REFERENCE NO.: 84:14673a,14676a
TITLE: A novel acetyl migration reaction from oxygen to oxygen in a pyridoxine derivative promoted by metal ions
AUTHOR(S): Iwata, Masaaki; Kuzuhara, Hiroyoshi; Emoto, Sakae
CORPORATE SOURCE: Inst. Phys. Chem. Res., Wako, Japan
SOURCE: Chemistry Letters (1976), (1), 17-18
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 2-Acetoxy-3-O-acetyl-4,5-O-isopropylidenepyridoxine (I, R = AcO) was converted to 2'-acetoxy-4'-acetylpyridoxine (III) in Me2CO in the presence of metal ions such as Zn, Cu, Fe, and Al. Of these catalysts Fe was the most effective. However, I (R = H) and its N-oxide did not give migration products with these catalysts.
IT 14213-49-1P 58620-81-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14213-49-1 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, acetate (ester) (8CI, 9CI) (CA INDEX NAME)




RN 58620-81-8 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, acetate (ester), 7-oxide (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:22040 CAPLUS
DOCUMENT NUMBER: 84:22040
ORIGINAL REFERENCE NO.: 84:3615a,3618a
TITLE: Pyridoxine derivatives. XIII. Hydrolysis of pyridoxine monooctanoates
AUTHOR(S): Mizuno, Nobuyasu; Fujimoto, Michiyo; Kamada, Akira
CORPORATE SOURCE: Fac. Pharm. Sci., Mukogawa Women's Univ., Nishinomiya, Japan
SOURCE: Bitamin (1975), 49(9-10), 395-401
CODEN: BTMNA7; ISSN: 0006-386X
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI For diagram(s), see printed CA Issue.
AB Pyridoxine 4-monooctanoate (I) [57547-09-8] was more soluble in organic solvents and water than pyridoxine 5-monooctanoate (II) [18426-21-6]. In buffer solns. of a constant pH between 2 and 3 hydrolysis of monooctanoates obeyed an apparent first-order kinetics. The substance passing through the rat intestine was pyridoxine [65-23-6] alone.
IT 57547-10-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57547-10-1 CAPLUS
CN Octanoic acid, 1,5-dihydro-3,3,8-trimethyl[1,3]dioxepino[5,6-c]pyridin-9-yl ester (CA INDEX NAME)

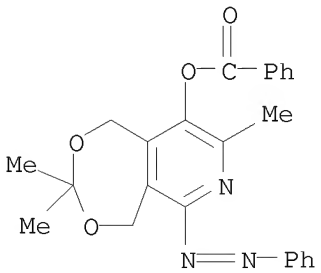


L5 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:511555 CAPLUS
DOCUMENT NUMBER: 79:111555
ORIGINAL REFERENCE NO.: 79:18067a,18070a
TITLE: Chemistry and biology of vitamin B6. 31. Synthesis and physicochemical and biological properties of 6-halogen-substituted vitamin B6 analogs
AUTHOR(S): Korytnyk, W.; Srivastava, S. C.
CORPORATE SOURCE: Dep. Exp. Ther., Roswell Park Mem. Inst., Buffalo, NY, USA
SOURCE: Journal of Medicinal Chemistry (1973), 16(6), 638-42
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

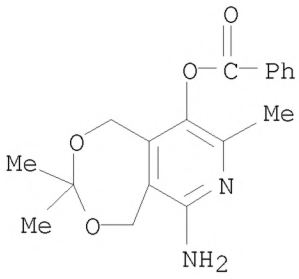
AB The presence of a 6-halogen atom in vitamin B6 analogs radically changed their phys.-chemical properties, especially pKa values, resulting in a loss of zwitterionic character and assumption of a hydrophobic character. All 6-fluoro analogs inhibited growth in vitro of mouse mammary adenocarcinoma and sarcoma 180 cells, the most potent compound being 6-fluoropyridoxal oxime (I) [42242-38-6], but were ineffective in the presence of 10-5 M pyridoxal [66-72-8]. I and 6-chloropyridoxol [15741-67-0] were potent convulsants in mice, causing 100% mortality at 50 and 100 mg/kg, resp. I was prepared from 6-aminopyridoxol [42242-40-0] by a modified Schiemann reaction yielding 6-fluoropyridoxol [42242-41-1], which was selectively oxidized with MnO2 to 6-fluoropyridoxal [42242-42-2] and treated with NH2OH.HCl. 6-Chloropyridoxol, the intermediate in preparation of chlorinated derivs., was prepared by chlorination of α4,α5-O-isopropylidenepyridoxol [948-00-5] with Me3COCl and acid hydrolysis. 6-Fluoropyridoxamine phosphate [42242-44-4] was a potent inhibitor in vitro of pyridoxine phosphate oxidase [9055-72-5], the enzyme catalyzing formation of pyridoxal phosphate.

IT 50441-56-0P 50441-57-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 50441-56-0 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-6-(phenylazo)-, benzoate (ester) (9CI) (CA INDEX NAME)



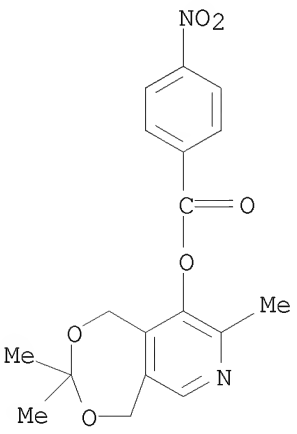
RN 50441-57-1 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 6-amino-1,5-dihydro-3,3,8-trimethyl-, benzoate (ester) (9CI) (CA INDEX NAME)


O
O
C
Ph
Me
O
Me
N
Me
O
NH2

L5 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:96571 CAPLUS
DOCUMENT NUMBER: 70:96571
ORIGINAL REFERENCE NO.: 70:18033a,18036a
TITLE: Pyridoxine chemistry. XX. Selective esterifications and acyl rearrangements in vitamin B6
AUTHOR(S): Paul, Burton; Korytnyk, Wsewolod
CORPORATE SOURCE: Roswell Park Mem. Inst., Buffalo, NY, USA
SOURCE: Tetrahedron (1969), 25(5), 1071-87
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 70:96571

AB Acyl migration and selective esterification were investigated in pyridoxal and pyridoxamine. Esterification of pyridoxal under various conditions gave esters with the hemiacetal structure. In pyridoxal, acyl migration could not be detected, possibly because of inability to form the ortho acid intermediate, hence permitting selective esterification of the phenolic hydroxyl. In pyridoxamine, O → N acyl migration takes place very readily from both the 3-O and α5-O positions, but the reverse migration could not be observed. 3-O,α4-N- and α4-N,α5-O-diesters of pyridoxamine were prepared Thus it is now possible to obtain selectively esterified derivs. of pyridoxal and pyridoxamine by taking advantage of either the absence or the presence of acyl migration. 5-Thiol esters of pyridoxol were obtained, but no acyl migration in the direction 5-S → 4-O could be detected. Factors that determine acyl migration are discussed.

IT 14210-78-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14210-78-7 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, 4-nitrobenzoate (ester) (9CI) (CA INDEX NAME)

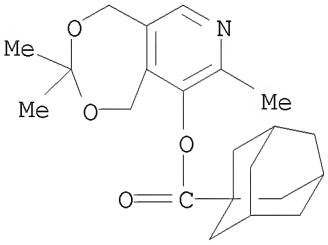


L5 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:402828 CAPLUS
DOCUMENT NUMBER: 69:2828
ORIGINAL REFERENCE NO.: 69:543a
TITLE: Pyridoxine chemistry. XVII. Adamantoyl esters of pyridoxol
AUTHOR(S): Korytnyk, W.; Fricke, G.
CORPORATE SOURCE: Roswell Park Mem. Inst., Buffalo, NY, USA
SOURCE: Journal of Medicinal Chemistry (1968), 11(1), 180-1
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Pyridoxal adamantoates having potential usefulness in probing for hydrophobic regions within the receptor sites at which pyridoxol analogs bind, are prepared in order to investigate the chemical and biol. usefulness of the adamantoyl group in vitamin B6 chemistry and pharmacology. The reaction of α4,3-O-isopropylidenepyridoxol (I) with adamantoyl chloride in pyridine gives α4,3-O-isopropylidene-α5-O-adamantoylpyridoxol (II), which when refluxed in HCl-MeOH yields α5-O-adamantoylpyridoxol-HCl (III). $$Graphic Adamantoylation of α4,α5-O-isopropylidenepyridoxol in pyridine with adamantoyl chloride gives α4,α5-O-isopropylidene-α3-O-adamantoylpyridoxal (IV), which rearranges in methanolic HCl to α4-O-adamantoylpyridoxol-HCl (V). Preliminary evaluation indicates that III and V are comparatively weak growth inhibitors.

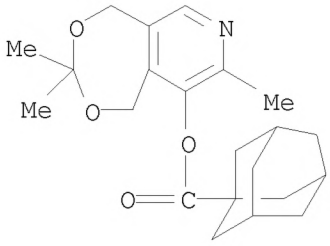
IT 18615-90-2P 18615-91-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18615-90-2 CAPLUS
CN 1-Adamantanecarboxylic acid, 3,3,8-trimethyl[1,3]dioxepino[5,6-c]pyridin-9-yl ester, hydrochloride (8CI) (CA INDEX NAME)




● HCl

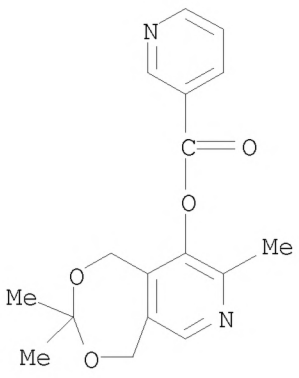
RN 18615-91-3 CAPLUS
CN 1-Adamantanecarboxylic acid, 3,3,8-trimethyl[1,3]dioxepino[5,6-c]pyridin-9-yl ester (8CI) (CA INDEX NAME)


Me
O
N
Me
Me
O
O
O
C

L5 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:69294 CAPLUS
DOCUMENT NUMBER: 68:69294
ORIGINAL REFERENCE NO.: 68:13411a,13414a
TITLE: Syntheses of nicotinic acid derivatives of amino acids, nucleosides, and vitamin B6 groups
AUTHOR(S): Uno, Hitoshi; Funabiki, Hiroko; Irie, Akira; Yoshimura, Yoshio
CORPORATE SOURCE: Dainippon Pharm. Co., Osaka, Japan
SOURCE: Yakugaku Zasshi (1967), 87(11), 1293-7
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB Amino acids, nucleosides, and vitamin B6 were treated with nicotinoyl chloride and the corresponding N-nicotinoyl derivs. were prepared Thus, 1 mole amino acid ester is dissolved in pyridine, stirred for 3 hrs. with 1 mole nicotinoyl chloride.HCl (Ia) to give the following N-nicotinoyl amino acids [structure, m.p., [α]D (c and solvent), and % yield given; Nic = nicotinoyl group]: DL-iso-PrCH(NHNic)CO2H (DL-I), 214-16°, -, 61; L-I, 222-4°, 15.7° (1.00, 50% EtOH), 33; L-iso-PrCH2CH(NHNic)CO2H, 185-7°, -6.2° (1.00, 50% EtOH), 20; NicNH(CH2)2CO2H, 157-9°, -, 12; L-PhCH2CH(NHNic)CO2H, 178-80°, -34.9° (1.00, 50% EtOH), 40; DL-MeS(CH2)2CH(NHNic)CO2H (DL-II), 216-18°, -, 56; L-II, 198-200°, -21.5° (1.00, 50% EtOH), 39; L-NicNH(CH2)3CH(NHNic)CO2H, 225-7°, -7.5° (1.00, 50% EtOH), 17; L-NicNH(CH2)4CH(NHNic)CO2H, 195-7°, -27.6° (1.05, H2O), 46; L-HO2CCH2CH(NHNic)CO2H, 185-7°, 15.04° [1.13, H2O], 36; L-HO2C(CH2)2CH(Nic)CO2Et, 163-5°, -22.5° (1.00, 50% EtOH), 2. Also prepared are the following nicotinoyl esters of nucleosides (name of the compound, m.p., and % yield given): 5'-O-nicotinoyladenosine, 135-40° (picrate m. 200-5°), 32; N6-2',3',5'-O-tetranicotinoyladenosine, 105-10°, 78; 2',3',5'-tri-O-nicotinoylguanosine, 160-80°, 43; 2',3',5'-tri-O-nicotinoylinosine, 178-81°, 78; 2',3',5'-tri-O-nicotinoylxanthosine, 175-80°, 40; trinicotinoyluridine, 177-8°, 48. Derivs. of vitamin B6 were also prepared Thus, 8.24 g. pyridoxine-HCl and 23.3 g. Ia are dissolved in 60 ml. CHCl3, 140 ml. pyridine is dropped in under icecooling, the whole stirred at room temperature for 3 hrs. to give 7.6 g. 3,α4,α5-tri-O-nicotinoylpyridoxine, m. 115-16.5°. Similarly prepared are: 3,α5-O-α4-N-trinicotinoylpyridoxamine (m. 174°), 3,α4-O-isopropylidene-α5-O-nicotinoylpyridoxine (m. 98-101°), α4,α5-O-isopropylidene-3-O-nicotinoylpyridoxine (m. 107-8.5°), α5-O-nicotinoylpyridoxine (m. 174-5°), α4,α5-di-O-nicotinoylpyridoxine (m. 112-13°), 6-methyl-7-nicotinoyloxy-1,3-dihydrofuro[3,4-c]pyridine (m. 163-5°), and 6-methyl-1,7-dinicotinoyloxy-1,3-dihydrofuro[3,4-c]pyridine (m. 118-19°).

IT 15922-83-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 15922-83-5 CAPLUS
CN Nicotinic acid, 1,5-dihydro-3,3,8-trimethyl[1,3]dioxepino[5,6-c]pyridin-9-yl ester (8CI) (CA INDEX NAME)


N
C
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O
Me
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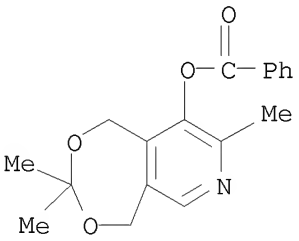
O

L5 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:28937 CAPLUS
DOCUMENT NUMBER: 68:28937
ORIGINAL REFERENCE NO.: 68:5575a,5578a
TITLE: Acyl migration and selective esterification in pyridoxol
AUTHOR(S): Korytnyk, Wsewolod; Paul, Burton
CORPORATE SOURCE: Roswell Park Mem. Inst., Buffalo, NY, USA
SOURCE: Journal of Organic Chemistry (1967), 32(12), 3791-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 68:28937

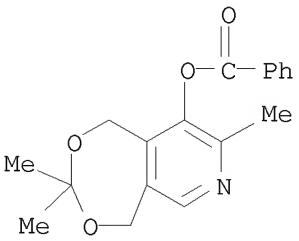
AB Acyl groups on the phenolic OH of pyridoxol migrated to the alc. OH in the 4-position. This rearrangement occurs with aromatic (benzoyl, p-nitrobenzoyl) and aliphatic (Ac, palmitoyl) esters. The mechanism of this rearrangement was studied. A rearrangement of this type takes place during partial esterification of pyridoxol with acid chlorides and explains the formation of aliphatic 3,4-diesters in high yields. 22 references.

IT 14210-76-5P 14210-77-6P 14210-78-7P
14213-49-1P 14213-50-4P 14320-31-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14210-76-5 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, benzoate (ester) (8CI, 9CI) (CA INDEX NAME)

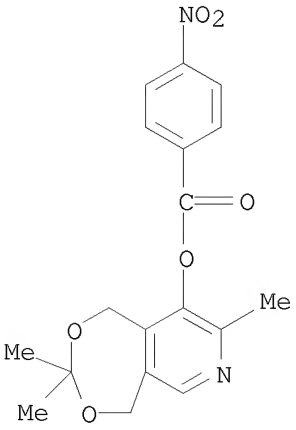


RN 14210-77-6 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, benzoate (ester), hydrochloride (8CI) (CA INDEX NAME)

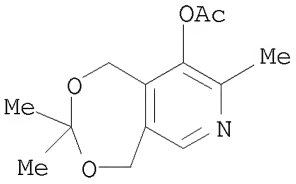


● HCl

RN 14210-78-7 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, 4-nitrobenzoate (ester) (9CI) (CA INDEX NAME)



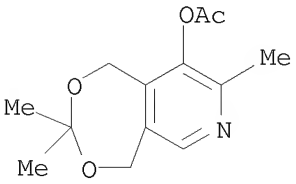
RN 14213-49-1 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, acetate (ester) (8CI, 9CI) (CA INDEX NAME)



RN 14213-50-4 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, acetate (ester), monopicrate (8CI) (CA INDEX NAME)

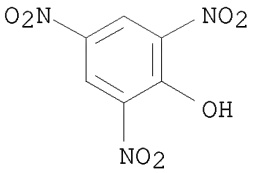
CM 1

CRN 14213-49-1
CMF C13 H17 N O4

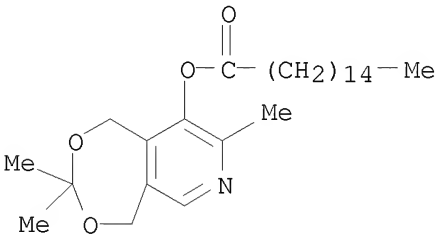


CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



RN 14320-31-1 CAPLUS
CN Palmitic acid, 1,5-dihydro-3,3,8-trimethyl-[1,3]dioxepino[5,6-c]pyridin-9-yl ester (8CI) (CA INDEX NAME)



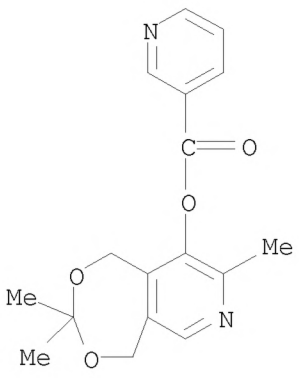
L5 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1967:482112 CAPLUS
DOCUMENT NUMBER: 67:82112
ORIGINAL REFERENCE NO.: 67:15479a,15482a
TITLE: Pyridoxinyl nicotinates
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd.
SOURCE: Neth. Appl., 18 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| NL 6608293 | | 19661216 | NL 1966-8293 | 19660615 |
| DE 1670526 | | | DE | |
| FR 5875 | | | FR | |
| GB 1149086 | | | GB | |
| JP 43014707 | | 19680000 | JP | |
| JP 44032412 | | 19690000 | JP | |
| US 3557131 | | 19710119 | US | 19660606 |
| PRIORITY APPLN. INFO.: | | | JP | 19650615 |
| | | | JP | 19651217 |

OTHER SOURCE(S): MARPAT 67:82112

AB The title compds., characterized by delayed activity of their components and hence having less side effects than nicotinic acid, are prepared The compds. also have hypocholesterolemic, anti-atherosclerotic, and hypoglycemic activity. Thus, a suspension of 2 g. pyridoxine-HCl and 5.3 g. nicotinoyl chloride-HCl in 50 ml. pyridine is agitated for 3 hrs., after which the mixture is filtered, the filtrate concentrated in vacuo, the residue dissolved in CHCl3, the CHCl3 solution washed, dried, and concentrated The residue is dissolved in EtOH, the solution saturated with dry HCl, diluted with Et2O, and the precipitate filtered, dissolved, and repptd. to give 1 g. 3,4,5-tri-O-nicotinoylpyridoxine, m. 173-5°. Similarly prepared are 3,5-di-O-nicotinoylpyridoxal, m. 118-19°; 3,5-di-O-nicotinoyl-4-N-nicotinoylpyridoxamine, m. 174°; 4,5-O-isopropylidene-3-O-nicotinoylpyridoxine, m. 107-8.5° (aqueous EtOH); 3,4-O-isopropylidene-5-O-nicotinoylpyridoxine, m. 98-101° (aqueous EtOH); 5-O-nicotinoylpyridoxine, m. 174° (EtOH).

IT 15922-83-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 15922-83-5 CAPLUS
CN Nicotinic acid, 1,5-dihydro-3,3,8-trimethyl[1,3]dioxepino[5,6-c]pyridin-9-yl ester (8CI) (CA INDEX NAME)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L5 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:424058 CAPLUS
DOCUMENT NUMBER: 63:24058
ORIGINAL REFERENCE NO.: 63:4263b-f
TITLE: Pyridine derivatives
INVENTOR(S): Kimel, Walter; Leimgruber, Willy
PATENT ASSIGNEE(S): F. Hoffmann-La Roche & Co., A.-G.
SOURCE: 7 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

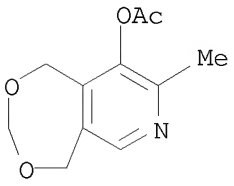
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| FR 1384099 | | 19650104 | FR 1963-954619 | 19631122 |
| BE 640507 | | | BE | |
| GB 1013893 | | | GB | |
| GB 1013894 | | | GB | |
| NL 301100 | | | NL | |
| US 3250778 | | 19660510 | US 1962-241019 | 19621129 |

PRIORITY APPLN. INFO.: US 19621129
GI For diagram(s), see printed CA Issue.
AB The known I, where R = alkyl, are prepared by acid hydrolysis from II in which R1 = H or acyl, R2 = H, alkyl, alkenyl, or aryl, R3 = H, alkyl, alkenyl, or aryl, or R2 and R3 = polymethylene. I and II form acid addition salts with inorg. or organic acids. II are obtained by condensation of 4,7-dihydro-1,3-dioxepins (III) with oxazoles (IV) where R4 is alkoxy or cyano at 80-250°. The intermediates V give II where R1 = H, or in the presence of alkylating agents, R1 = alkoxy. The reaction of III with IV is catalyzed by acids and autocatalyzed by II. The intermediate II need not be isolated. II, V, and some III are new. Thus, a mixture of 300 g. cis-2-butene-1,4-diol, 31. acetone, 200 g. Na2SO4, and 13 ml. concentrated H2SO4 kept 20 hrs. gives III (R2 = R3 = Me), b755 144.5-47°, n24.5D 1.4465. III (R2 = R3 = H) (2.4 g.), 2.1 g. IV (R = Me, R4 = CN) and CCl3CO2H in a sealed tube at 150° for 20 hrs. gives II (R = Me, R1 = R2 = R3 = H) (VI), m. 175-6°; hydrochloride m. 208-8.5°. VI with Ac2O then ethanolic HCl gives hydrochloride of II (R = Me, R1 = Ac, R2 = R3 = H) (VII), m. 194-5°; free base m. 86.5-7.5°. VII refluxed with 12N methanolic HCl 16 hrs. gives I (R = Me) hydrochloride, m. 207-8° (decomposition). VI (50 mg.) with 5 ml. AcOH, 1 ml. H2O, and 0.1 ml. 72% HClO4 refluxed 3 hrs., evaporated, and crystallized from ethanolic HCl gives I (R = Me) hydrochloride, m. 208-9° (decomposition). Also prepared were II (R = Me, R1 = R2 = H, R3 = iso-Pr), m. 164-4.5° [(HCl salt m. 190-1° (decomposition); acetate-HCl (VIIa) m. 173-3.5°], II (R = Me, R1 = R2 = H, R3 = Ph) (VIIb), m. 160-60.5°, II [R = Me, R1 = H, (R2R3 = ) (CH2)5] (VIII), m. 167-9° (in vacuo). IV (R = Me, R4 = MeO) b. 140-2°. VIII (100mg.) and 10 ml. N/HCl heated on a steam bath 15 min. gave pyridoxol-HCl, m. 202-3° (decomposition), also prepared from VIIa, VIIb, and VII, and from 4-methyloxoazole-5-carbonitrile (IX) and 4,7-dihydro-2-isopropyl (or phenyl)-1,3-dioxepin. IX (3 ml.) and 25.2 g. 4,7-dihydro-2-propenyl-1,3-dioxepin (X) heated 17 hrs. at 180° in a sealed tube to give II (R = Me, R1 = R3 = H, R2 = propenyl), which treated with alc. HCl gave pyridoxol-HCl, similarly prepared from IX and the 2,2-dimethyl analog of X.
IT 1622-66-8P, [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-8-methyl-, acetate 1966-88-7P, [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3-isopropyl-8-methyl-, acetate, hydrochloride 2319-67-7P, [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-8-methyl-, acetate, hydrochloride

RL: PREP (Preparation)
(preparation of)

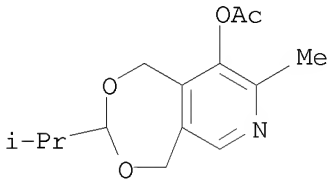
RN 1622-66-8 CAPLUS

CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-8-methyl-, acetate (ester) (9CI) (CA INDEX NAME)




RN 1966-88-7 CAPLUS

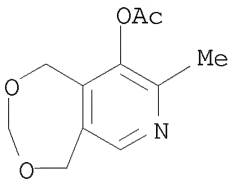
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3-isopropyl-8-methyl-, acetate (ester), hydrochloride (8CI) (CA INDEX NAME)




● HCl

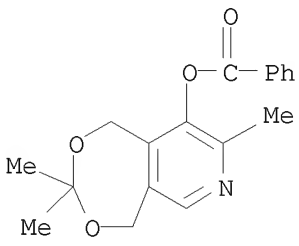
RN 2319-67-7 CAPLUS

CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-8-methyl-, acetate (ester), hydrochloride (9CI) (CA INDEX NAME)




● HCl

L5 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:33247 CAPLUS
DOCUMENT NUMBER: 58:33247
ORIGINAL REFERENCE NO.: 58:5622h,5623a-c
TITLE: Seven-membered cyclic ketal of pyridoxol
AUTHOR(S): Korytnyk, W.
CORPORATE SOURCE: Roswell Park Mem. Inst., Buffalo, NY
SOURCE: Journal of Organic Chemistry (1962), 27, 3724-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:33247
GI For diagram(s), see printed CA Issue.
AB Pyridoxol-HCl (I) (12 g.) suspended in 300 ml. Me2CO treated in the cold with dry HCl 25 min. (13 g. HCl taken up), the mixture shaken 1 hr., kept overnight at -10 to -20°, and filtered, the mixture (10 g.) suspended in K2CO3 solution and kept several hrs. at 5°, and the product crystallized gave 5.4 g. α4,α5-O-isopropylidenepyridoxol (II), m. 184-5° (aqueous MeOH). I (12 g.) suspended in 250 ml. Me2CO treated in 5 min. with 11 g. dry HCl gave 74% crude II. II (0.245 g.) in N HCl heated 40 min. at 85-90° gave 0.225 g. I, m. 210-12° (decomposition). II (2.415 g.) in 50 ml. C5H5N treated 2 hrs. at 0° with 2.5 ml. BzCl gave 3.23 g. 3- O-benzoyl-α4,α5-isopropylidenepyridoxol, m. 107-9° (aqueous alc.). II (1.05 g.) in 50 ml. C5H5N treated 16 hrs. at room temperature with 2.23 g. p-MeC6H4SO2Cl gave 1.45 g. 3-O-p-toluenesulfonyl-α4,α5-O-isopropylidenepyridoxol (III), m. 145-6°. 3-O-Methanesulfonyl-α4,α5-O-isopropylidenepyridoxol, similarly obtained, m. 72-3°. III (0.9 g.) heated 0.5 hr. with 100 ml. 10% HCO2H containing 20 ml. alc. gave 0.63 g. 3-O-p-toluenesulfonylpyridoxol, m. 186-7° (CHCl3-alc.). II was stable to alkali. In contrast to the 6-membered ketal II could be readily monotosylated and monomesylated as shown above. Comparison of the ultraviolet spectra of II, pyridoxol, and α4-3-O-isopropylidenepyridoxol confirmed the structure of II.
IT 14210-76-5P, [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, benzoate
RL: PREP (Preparation)
(preparation of)
RN 14210-76-5 CAPLUS
CN [1,3]Dioxepino[5,6-c]pyridin-9-ol, 1,5-dihydro-3,3,8-trimethyl-, benzoate (ester) (8CI, 9CI) (CA INDEX NAME)



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FULL ESTIMATED COST                                      96.69     275.26

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CA SUBSCRIBER PRICE                                     -13.60     -13.60

FILE 'STNGUIDE' ENTERED AT 13:03:42 ON 04 APR 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 28, 2008 (20080328/UP).

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SOME IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
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=> log y
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FULL ESTIMATED COST                                       1.32     276.58

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